



A New Approach to Propellant Formulation: Minimizing Life-Cycle Costs Through Science-Based Design

by Martin S. Miller, Betsy M. Rice, Anthony J. Kotlar,
and Randall J. Cramer

ARL-TR-2291

August 2000

Approved for public release; distribution is unlimited.

The findings in this report are not to be construed as an official Department of the Army position unless so designated by other authorized documents.

Citation of manufacturer's or trade names does not constitute an official endorsement or approval of the use thereof.

Destroy this report when it is no longer needed. Do not return it to the originator.

Army Research Laboratory

Aberdeen Proving Ground, MD 21005-5066

ARL-TR-2291**August 2000**

A New Approach to Propellant Formulation: Minimizing Life-Cycle Costs Through Science-Based Design

Martin S. Miller, Betsy M. Rice, and Anthony J. Kotlar
Weapons and Materials Research Directorate, ARL

Randall J. Cramer
Naval Surface Warfare Center, Indian Head Division

Abstract

The traditional approach to developing propellants for specific gun applications relies heavily on trial and error. Candidate formulations must be made in small quantities and subjected to burning-rate measurements and small-scale vulnerability assessments. If the properties of these candidates fail to meet expectations, the process must be repeated. This approach, while historically unavoidable, is obviously inefficient in time and expense and can generate considerable waste streams associated with unsuccessful formulations. With added considerations of life-cycle costs, including environmental impact at all stages of development, use, and disposal, this traditional approach becomes increasingly unworkable. This report proposes a new approach that makes maximal use of scientific understanding embodied in models during the early phases of the propellant-development cycle. Simple simulations show that this strategy can have a significant impact on the overall costs of the development process. In analogy to the Department of Energy (DOE) program to convert the nuclear-weapon stewardship from testing-based to science-based, we term the new approach science-based design. This new approach will require concentration and leveraging of resources toward the most critical early-phase development steps; with the reality of declining resources, it may be the only credible strategy to reconcile the need for higher-performance weapons.

Acknowledgments

This work was supported by the Strategic Environmental Research and Development Program (SERDP) under Project CPO/8. The authors wish to thank Dr. Douglas Kooker and Ronald Anderson for helpful discussions.

INTENTIONALLY LEFT BLANK.

Table of Contents

	<u>Page</u>
Acknowledgments	iii
List of Figures	vii
List of Tables	ix
1. Introduction	1
2. Traditional Propellant-Formulation Process	2
3. The Impact of Life-Cycle Analysis on Propellant Formulation	6
4. Propellant Formulation Through a Science-Based Approach	7
5. Implementation	11
6. References	21
Distribution List	23
Report Documentation Page	31

INTENTIONALLY LEFT BLANK.

List of Figures

<u>Figure</u>	<u>Page</u>
1. Conventional Procedure for Development of a New Propelling Charge for Guns	4
2. Conventional Procedure for Developing a Propelling Charge With the Addition of Two New Loops (2 and 6) Recognizing Environmental Constraints	8
3. Streamlined Propelling-Charge Development Utilizing Modeling During Early Phases	12
4. Flow Chart Illustrating the Progressive Winnowing of Propellant Candidates Through a Hierarchy of Models of Increasing Sophistication	15
5. Simplification of Propelling-Charge Development Possible With Full Implementation of Science-Based Design	17

INTENTIONALLY LEFT BLANK.

List of Tables

<u>Table</u>	<u>Page</u>
1. Demonstration of the Multiplier Effect Associated With Repetitive Executions of Low-Cost, Inner-Loop Steps in Traditional Propellant-Formulation Procedure of Figure 1	6
2. Effect on the Total Cost of Development of Including Two Environmental Steps Into the Traditional Propellant-Formulation Procedure	9
3. Effect of Streamlining the Propellant-Formulation Procedure Through the Use of Modeling and Simulation	13
4. Identification of Codes Used in Figure 4	16

INTENTIONALLY LEFT BLANK.

1. Introduction

The recent Quadrennial Defense Review [1] discussed the challenges faced by the Department of Defense (DOD) in realizing the new support structure needed to achieve the future military forces outlined in the Joint Vision 2010 document [2]. In order to afford the increasing expenditures associated with these new capabilities, the QDR concluded that support operations must be "leaner, more efficient, and more cost effective. We not only have the opportunity to change, we have the requirement to change." Nowhere is this mandate more apt than in the development of new propellant formulations for advanced munitions. In the past, development has been dependent on trial and error approaches, which are costly, inefficient, and time consuming. Compounding these problems are new environmental guidelines and constraints with which future development programs must comply. Since conventional propellant development and manufacture produces large amounts of waste, these new requirements could hobble the process. During the development of XM39 gun propellant during the 1980s, for example, about 50,000 lb of test material was produced [3], almost all of which was waste resulting from the trial and error testing required. During the current manufacture of M30 gun propellant, an estimated 0.3 lb of ethanol and acetone are released to the atmosphere for every pound of propellant [4]. These examples hint at the scale of potential environmental hazards that now must be addressed. As more performance is demanded from gun systems, the margin for error in their design decreases, leading to even greater levels of trial and error during development. Clearly, the added modern burden of environmental responsibility will render the traditional approach to propellant development even more unmanageable.

The new environmental constraints are not trivial add-on requirements. They encompass the manufacture of every ingredient, fabrication of the propellant itself, emissions in training and deployment, stability during storage, and demilitarization when no longer useful. Design foresight on issues relating to storage (stability surveillance and emissions) are of great potential importance since the useful life of propellants can be long; 16-in naval guns, for instance, still use a propellant known as pyro, which was manufactured during (or just after) World War II. Propellants are also manufactured in large quantities; a single batch of artillery propellant is typically more than a hundred thousand pounds. Thus, the cradle-to-grave costs associated with propellants, both to the

national treasury and to the environment, are potentially very substantial. While assessing life-cycle costs for a new propellant is difficult, managing these costs using the traditional trial and error development method is all but impossible. It is argued in this report that the conflict between the need to develop advanced propellants for more lethal, survivable weapons and the need to minimize life-cycle costs can be resolved only by a new approach. Just as new realities have forced the maintenance of the nation's nuclear stockpile to pass from a testing-based to a science-based approach, developing new propellants must transition from a trial-and-error-based to a science-based approach.

Fortunately, the scientific understanding of the microscopic processes involved in the structure and combustion of energetic materials has seen great progress over the last decade. Although this understanding is far from complete, sufficient progress has been made to permit a vision of how new tools for the smart design of propellant formulations might be used to minimize inefficiencies in the propellant formulation process. Such an exercise is also valuable in identifying those key aspects of the problem where investments in future scientific understanding might be made most profitably. The ideal developmental process utilizing these emerging technologies will incorporate the constraint of reducing the waste streams resulting from all the stages of fielding a new propellant with preserving the given performance objectives, which are the *raison d'être* for the process. This report will outline such a streamlined development approach.

2. Traditional Propellant-Formulation Process

The traditional procedure for formulating new propellants, guided largely by intuition, experience, and testing, relies heavily on trial and error. Candidate propellant mixes must be made and subjected to a sequence of tests, many of which generate hazardous emissions and wastes. In addition to the waste generation associated with test and evaluation, many of the candidates are discarded from further consideration due to unacceptable levels of performance or other problems that arise in the qualification procedure. For these cases, waste costs accrue for unsuccessful formulations, synthesis and testing, and disposing of any excess material. It is clear that such cut-and-try approaches, although previously unavoidable, are now considered inefficient, costly, and environmentally undesirable.

Figure 1 illustrates the conventional process of developing a new propelling charge. This flow chart presumes that adequate ingredients (e.g., energetic materials and polymeric binders) are "on the shelf" to achieve a successful formulation. If this is not the case, then new ingredients with the desired characteristics must be developed. Before embarking on the procedure outlined in Figure 1, the weapons designer will have specified his requirements, which in the past have been driven mainly by performance or vulnerability requirements. The initial screening represented by Loop 1 consists of computations of impetus, flame temperature, and idealized maximum performance based on thermodynamic equilibrium, which may be viewed as a limiting case. At this stage, a formulation can be rejected if it cannot meet performance needs, even assuming a theoretical maximum performance. If a candidate passes this level, however, shortfalls from theoretically ideal performance revealed at subsequent levels may yet cause it to be rejected, in which case the burden falls back on the formulator to provide a new candidate to run the gauntlet of screening tests from the beginning. (Note: In this flow chart and those to follow, a very complex process is rationalized into a limited number of discrete steps. Such an idealization is necessarily oversimplified and is intended to serve only a heuristic purpose.)

Once the small-scale evaluations are made, then more extensive tests and measurements are performed for increasingly larger samples. As evident in this figure, the conventional method has a notable degree of physical testing and measurement, which could generate a significant amount of waste. Although the small-scale screening procedures contained within the first four loops are relatively inexpensive on a per-sample basis in terms of time, material, and equipment requirements, these might become quite cost intensive if a series of failures require reformulating and retesting several candidates. Because of the nested nature of these screening loops, an inexpensive single-step operation could make the formulation procedure cost prohibitive.

As an illustration of the potential expense associated with the repeated execution of the innermost loops resulting from the traditional trial and error approach to propellant formulation, consider the following fictitious case of a gun-propellant development. To determine the expense associated with developing a new propelling charge, costs were assigned to each stage of the formulation procedure outlined in Figure 1. Naturally, these costs will vary enormously in

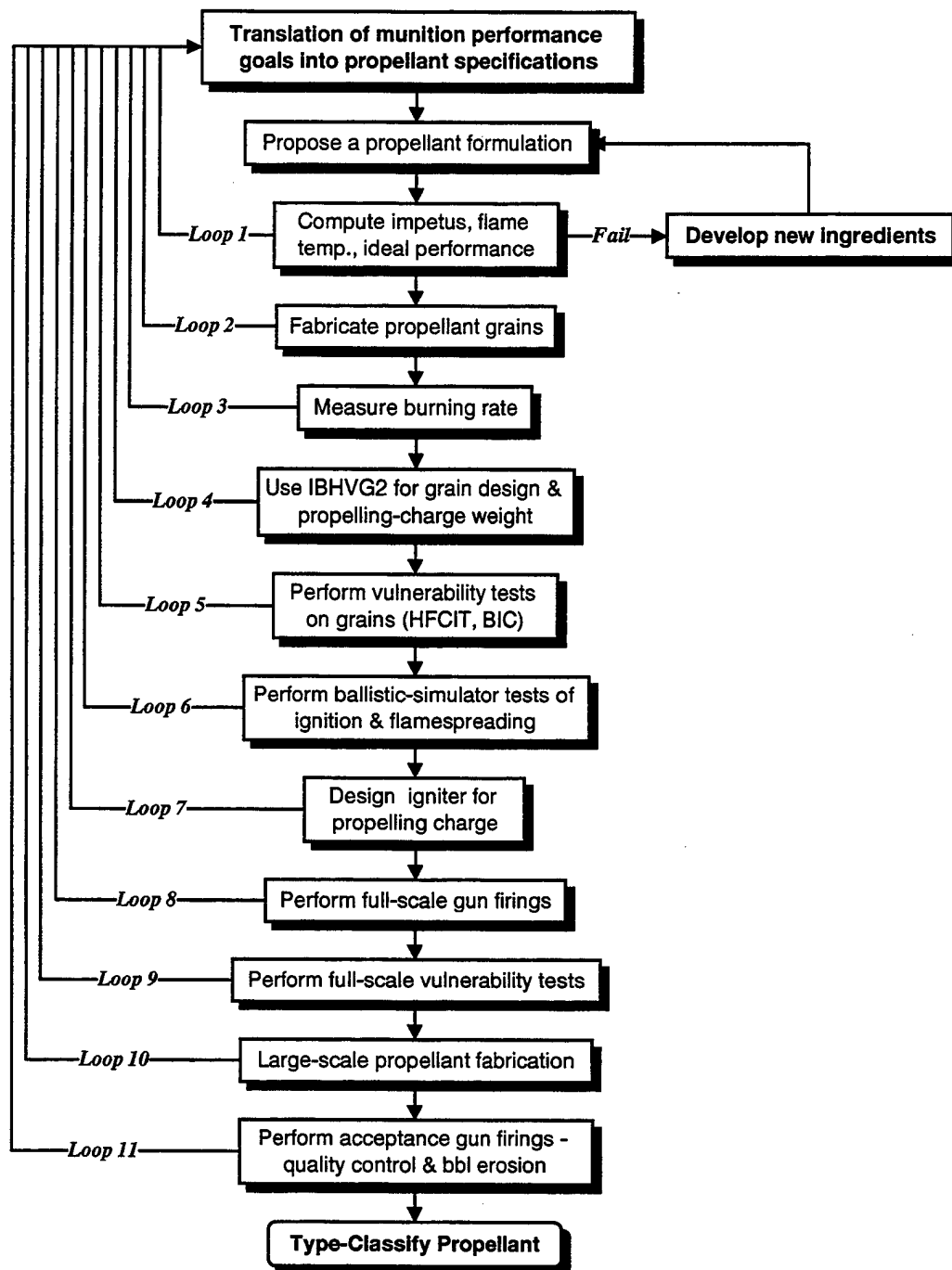


Figure 1. Conventional Procedure for Development of a New Propelling Charge for Guns.

actual cases, but an effort was made to make reasonable estimates for these steps. These numbers should be taken within their intended heuristic context and not taken literally. The relative values assigned are intuitively reasonable in that the early “screening” processes are the least expensive, and

the large-scale processes reflect the more significant costs of the procedure. For the purposes of this illustration, it was assumed that the formulator did not require new energetic material synthesis.

In this exercise, it was assumed that the progression through the entire process would require three passes through each loop in Figure 1. In reality, of course, each loop will incur a different number of executions uniquely specific to each propellant-development case. The value of choosing a single number for all loops is purely in the simplicity and transparency it confers to the simulation. The selected value of three passes is arbitrary, but it reflects the reality of at least some degree of trial and error.

The results of this simulation are given in Table 1. In this simple example, three-fourths of the total cost occurs in the first three stages of the developmental process through steps that, when individually taken, are at three to four orders of magnitude less expensive than the processes near the end of the developmental process. This result is dramatic evidence of the enormous hidden costs associated with trial-and-error testing at the early development stages. In actual practice, the total costs incurred by this inner-loop testing have never been this large, only because a complete matrix of testing would be prohibitive. The thoroughness of the formulation search was therefore consciously curtailed. Undoubtedly, the incompleteness of the search jeopardizes optimization of the formulation. Another reason that such inner-loop costs have never been this large is that performance requirements would have been sacrificed at an early stage to keep costs down. This downgrading of expectations could have easily compromised the maximum attainable performance had more complete testing been feasible.

The inefficiencies inherent in the trial-and-error approach may have consequences beyond exorbitant monetary cost. In the modern era of warfare, a great premium is placed on agile response capability to new threats. There could be occasions where protecting some strategic asset is worth virtually any expenditure, yet the time needed to extensively test may prove to be the pacing limitation. An example of the time needed to develop a new propellant can be seen in the case of M43, a high-performance tank-gun propellant. M43 was under development for almost 20 years before being type classified shortly before Operation Desert Storm. In this case, the presence of an untried propellant ingredient, cyclotrimethylenetrinitramine (RDX), may have materially lengthened

Table 1. Demonstration of the Multiplier Effect Associated With Repetitive Executions of Low-Cost, Inner-Loop Steps in Traditional Propellant-Formulation Procedure of Figure 1

Loop No.	Per-Loop Cost (\$K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed \times Cost/Loop) (\$K)
1	3	$3^{11} = 177,147$	531,441
2	5	$3^{10} = 59,049$	295,245
3	2	$3^9 = 19,683$	39,366
4	5	$3^8 = 6,561$	32,805
5	5	$3^7 = 2,187$	10,935
6	40	$3^6 = 729$	29,160
7	10	$3^5 = 243$	2,430
8	300	$3^4 = 81$	24,300
9	100	$3^3 = 27$	2,700
10	3,000	$3^2 = 9$	27,000
11	50,000	$3^1 = 3$	150,000
Total Cost			1,145,382

the process. But instead, this lack of experience simply increased the number of iterations of testing needed to assure the safety and consistency of the new propellant. Obviously, there may likewise be cases where the environmental consequences of a particular propellant or ingredient may be so egregious that cost and time become of secondary importance.

3. The Impact of Life-Cycle Analysis on Propellant Formulation

The need to minimize the waste associated with the propellant formulation process is no longer driven purely by monetary constraints. Environmental restrictions and requirements have demanded

that environmental impact be given equal or greater weight in the development and design of a new gun propellant. Along with increasingly important environmental considerations has come a focus on the true cradle-to-grave costs of weapons systems. Optimizing the design of a system to minimize development, manufacturing, and operational costs is a considerable challenge. Now, the cost of demilitarizing the system at the end of its useful life must also be included. In the past, propellants have been disposed of by open-air burning. In the future, this method of disposal may not be allowed. Therefore, considering how the propellant will eventually be destroyed or recycled will have to be included in its design. The collective cradle-to-grave costs, including environmental considerations at each stage of manufacture, use, and disposal, have been termed life-cycle costs.

To account for these requirements, the propellant formulation procedure must be modified to reflect these new design considerations. Figure 2 suggests how the inclusion of environmental constraints (Loops 2 and 6) might modify the conventional propellant-development flow chart (Figure 1). The simulation logic of Table 1 assists in estimating the added burden on the propellant development process introduced by the environmental considerations. In the modified simulation shown in Table 2, very modest per-loop costs are assigned to the environmental steps. A substantial increase in total cost results from adding only two new steps. Even if it is assumed that these two environmental steps cost nothing, the total cost of the development sequence is increased by a factor of five. Obviously, adding environmental constraints can easily overwhelm the practicality of the traditional cut-and-try development method. Greater rationalization of the early steps in the propellant-development procedure is clearly needed to successfully manage this added complexity.

4. Propellant Formulation Through a Science-Based Approach

Prior to the ban on underground nuclear weapon tests, the Department of Energy (DOE) used direct tests to regularly test design concepts and the safety and reliability of nuclear weapons in the strategic stockpile. With the cessation of testing, these concerns had to be satisfied through computation based on a reliable scientific understanding. This strategy is embodied in what is called

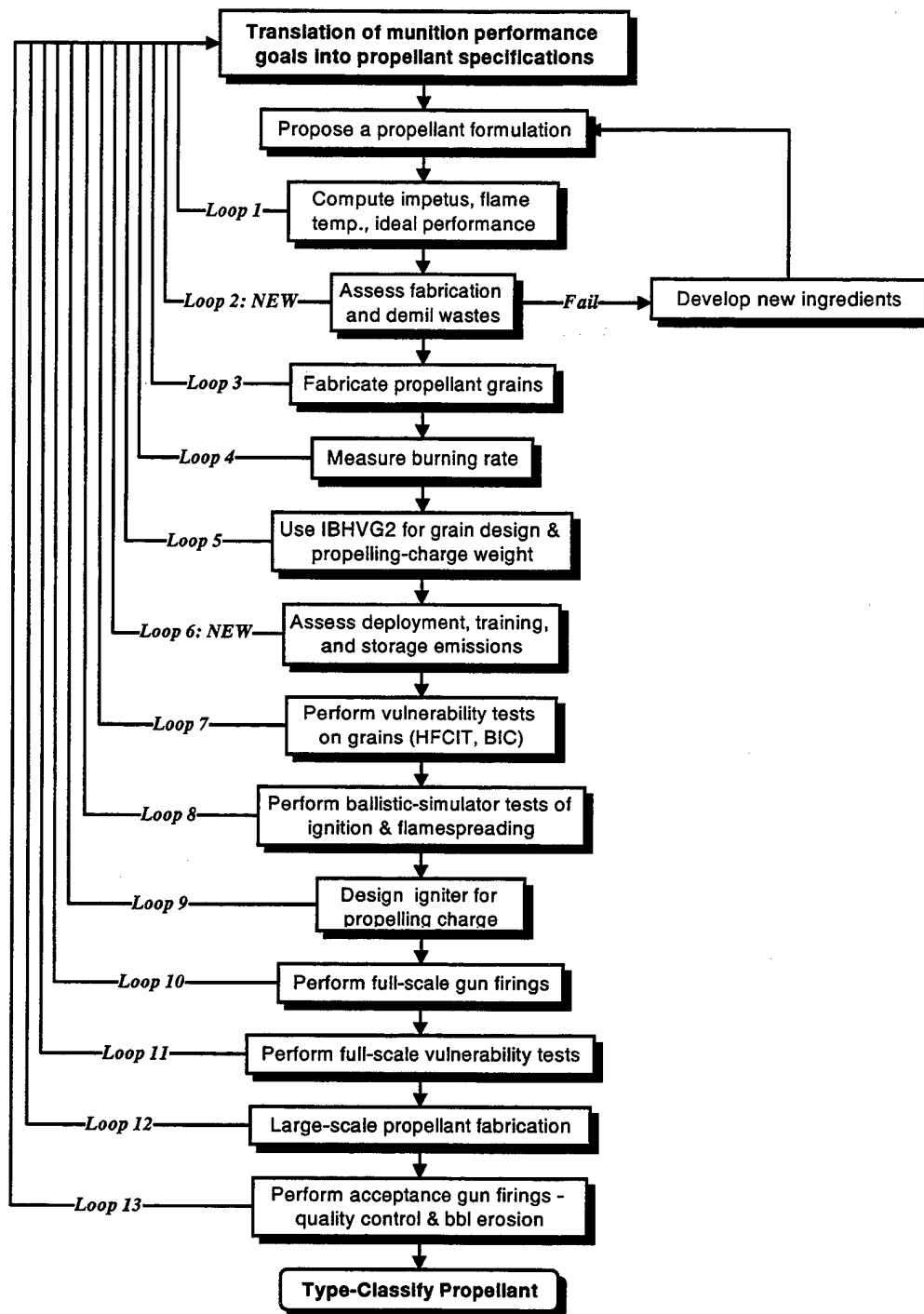


Figure 2. Conventional Procedure for Developing a Propelling Charge With the Addition of Two New Loops (2 and 6) Recognizing Environmental Constraints.

Table 2. Effect on the Total Cost of Development of Including Two Environmental Steps Into the Traditional Propellant-Formulation Procedure (Figure 2)

Loop No.	Per-Loop Cost (\$K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed \times Cost/Loop) (\$K)
1	3	$3^{13} = 1,594,323$	4,782,969
2	2	$3^{12} = 531,441$	1,062,882
3	5	$3^{11} = 177,147$	885,735
4	2	$3^{10} = 59,049$	118,098
5	5	$3^9 = 19,683$	98,415
6	4	$3^8 = 6,561$	26,244
7	5	$3^7 = 2,187$	10,935
8	40	$3^6 = 729$	29,160
9	10	$3^5 = 243$	2,430
10	300	$3^4 = 81$	24,300
11	100	$3^3 = 27$	2,700
12	3,000	$3^2 = 9$	27,000
13	50,000	$3^1 = 3$	150,000
Total Cost			7,220,868

a science-based stewardship. This term is not meant to imply that science was not formerly used; however, now the burden to assure an accurate, detailed understanding of the microscopic processes is acute, as total reliance is being placed on it. The DOE has redirected funds formerly used in testing into experiments and theory designed to bolster gaps in fundamental understanding of phenomena related to design and aging issues. While testing in the development of propellants is permissible and important, it is expensive in dollars, time, and environmental impact. The propellant-formulation community could profitably adopt the spirit of the DOE science-based strategy.

Efforts to develop predictive technologies leading to smart design have been underway for several years within DOD mission programs. These efforts include developing molecular-dynamic models [5–7] of RDX (and CL20) structure and aggregate properties, theoretical tools [8] for predicting the stability and heats of formation for notional energetic materials, models [9] to predict the burning rate of a propellant from its ingredients, and models [10, 11] to compute the effects of finite-rate kinetics on flame spreading in a propelling charge. These emerging predictive technologies can form the basis of the science-based approach to propellant development, which can in turn minimize the cost of the propellant formulation procedure by reducing synthesis and measurement. Unfortunately, these efforts have focused almost solely on performance, without regard to environmental hazard. A continued and leveraged effort to develop these capabilities to incorporate environmental constraints should be undertaken.

To minimize propellant-development costs (whether they be monetary, time, or environmental), the developmental procedure must be optimized. Such an optimization can be achieved if:

- (1) the number of times the inner loops are accessed is minimized, and
- (2) the processes included in inner loops are either eliminated or made as cost efficient as possible.

These two requirements for achieving optimization can be met by extensively utilizing modeling and simulation. Results from modeling and simulation provide the insight needed for the smart design of materials. Modeling and simulation are relatively cheap and fast. There is no need to fabricate test material and no need for the labor and expense of manning and maintaining test equipment. Additionally, there is no expense associated with hazardous material, including synthesis, handling, cleanup, or disposal costs.

Figure 3 shows a flow diagram attempting to optimize the propellant formulation procedure by replacing early-phase testing and measurement with modeling and simulation. Continuing in the spirit of the two simulations previously mentioned, it was assumed that a model for predicting the

burning rate has been developed and that it was incorporated into Loop 1. The capability to compute the burning rate would obviate the need for fabricating propellant grains for the burning rate measurement and the measurement itself. Next, it was assumed that vulnerability models exist that can at least screen candidates at the Loop 1 level. Finally, it was assumed that models exist that can predict flame spreading and igniter functioning well enough to eliminate the testing associated with these steps and incorporate these functions into Loop 4. The per-loop execution cost in Loops 1 and 4 was increased to reflect the added modeling effort. These activities are all areas of active research under mission programs of the U.S. Army Research Laboratory (ARL) and have realistic chances for success.

The results of this simulation are given in Table 3, and they show a dramatic drop in total development costs by a factor of almost 30. Notice that the new emphasis on smart design returns the heaviest cost burden to the large-scale testing and acceptance firings. Concern over troop safety will always demand extensive quality assurance testing at this end of the development cycle. Modeling and simulation are most effectively used in the beginning stages of the development cycle. These numbers are not intended to be taken too literally. The total costs are obviously a function of the number of steps in each chart, and the degree of simplification inherent in these charts does not permit them to be unique. On the other hand, the concept behind the numbers is sound. Adding environmental constraints unambiguously adds steps to the development process, which increases costs. Innermost loop functions are exercised the most and are the most susceptible to having testing replaced by models. Replacing relatively expensive testing with relatively inexpensive models leads to either total elimination of inner-loop steps (such as propellant fabrication for burning-rate tests) or consolidated inner-loop functions. The end result is an unambiguous reduction in money, time, and environmental impact.

5. Implementation

The simplified flow charts illustrate the nested-loop nature of the propellant-development process and the total cost reduction that will be realized by modeling various combustion characteristics and

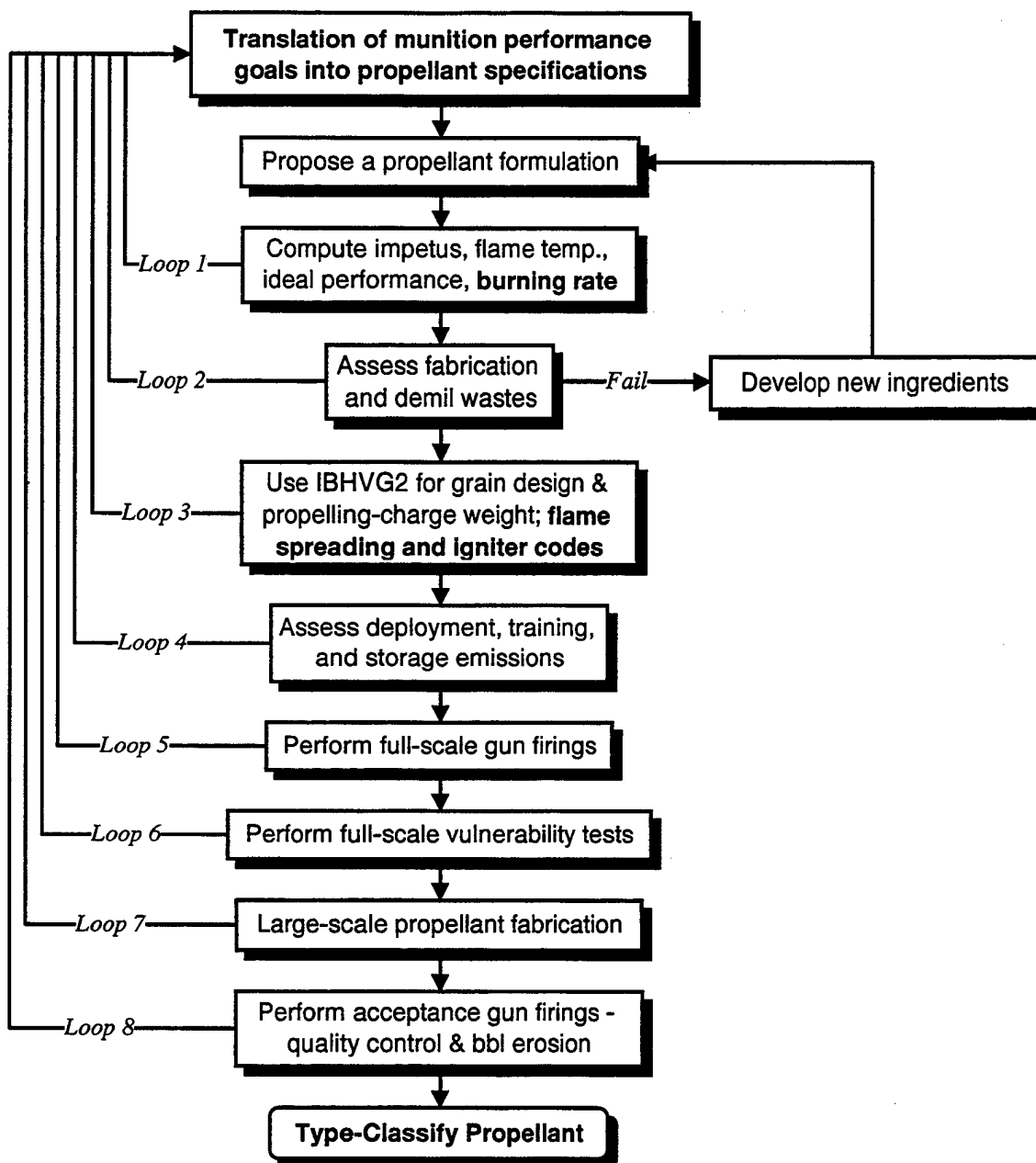


Figure 3. Streamlined Propelling-Charge Development Utilizing Modeling During Early Phases.

Table 3. Effect of Streamlining the Propellant-Formulation Procedure Through the Use of Modeling and Simulation (Figure 3)

Loop No.	Per-Loop Cost (\$K)	Total No. of Times Executed During Entire Procedure	Total Cost of This Step Through Entire Procedure (Total No. of Times Executed \times Cost/Loop) (\$K)
1	5	$3^8 = 6,561$	32,805
2	2	$3^7 = 2,187$	4,374
3	7	$3^6 = 729$	5,103
4	4	$3^5 = 243$	972
5	300	$3^4 = 81$	24,300
6	100	$3^3 = 27$	2,700
7	3,000	$3^2 = 9$	27,000
8	50,000	$3^1 = 3$	150,000
Total Cost			214,449

behavior. They do not, however, convey the fact that a hierarchy of models exist with differing sophistication and differing requirements for the input information. For example, IBHVG2 is an interior-ballistic code useful in the preliminary design of a propelling charge, but it cannot predict problems with ignition delays arising from finite-rate chemical kinetics. On the other hand, it also does not require chemical kinetic mechanisms as input, as would the more sophisticated XNOVAKTC/NGEN codes. The XNOVAKTC/NGEN codes also consume considerably greater computer resources and require more skill to use properly. Thus, for the optimum candidate, the most efficient approach to sorting through a large number of existing propellants is to use a succession of codes of increasing sophistication. Eliminate as many candidates as possible by using simpler codes first; reserve the more detailed, data-hungry, and operator-intensive codes for the more promising candidates. A flow diagram illustrating this hierarchy of sophistication in evaluation codes is given in Figure 4. References for the computer codes identified in Figure 4 are given in Table 4.

In Figure 4, the first set of models labeled “preliminary screening models” are the least sophisticated models—they require the least extensive input data and are therefore expected to produce the least accurate results. To prevent the rejection of good candidates because of inaccuracies in these models, candidates at this level should be eliminated according to the least strict screening tolerances. As the sophistication (and hence accuracy) improves with the intermediate and advanced evaluation models, the screening tolerances represented by the diamond shapes would likewise decrease appropriately.

A parallel demonstration study [12] used the logic embodied in Figure 4 (preliminary screening and intermediate evaluation models only) to identify the best existing gun propellant for a real gun system with user requirements. In this work, the user-supplied requirements included the maximum pressure limitation and minimum muzzle energy required by a propelling charge for a Navy 5-in, 54-cal. gun. A candidate set of 10 existing propellant formulations representing single, double, triple-based, and composite nitramine propellants was used for the down-select procedure. All combustion properties of this list of propellants are known. The procedure began by assessing environmentally unacceptable ingredients in the propellants—this eliminated two candidates. Thermodynamic property information was obtained from existing literature to assess ideal performance (i.e., muzzle velocity assuming constant maximum pressure during the firing). These estimates allowed a further culling of candidates. Additional unsuccessful candidates were eliminated from the next stage of screening, which is a calculation of interior ballistics performance assuming propellant grain design. At the end of the exercise, the user was left with only a few candidates for further study. At this stage, users can rank these candidates according to their specifications, and more advanced models can be employed to make the final suitability assessment. Thus, this exercise illustrated how the procedure outlined in Figure 4 can be used to reduce the waste stream in the formulation process, while continuing to meet the performance objectives for the gun.

The task now remains to transition this procedure from an idealized concept into a working methodology. Each of the boxes in Figure 4 represent an opportunity to perform a theoretical analysis in lieu of more costly testing. Many of the models described are under development; however, there are many more that need to be developed. For example, the success of the parallel

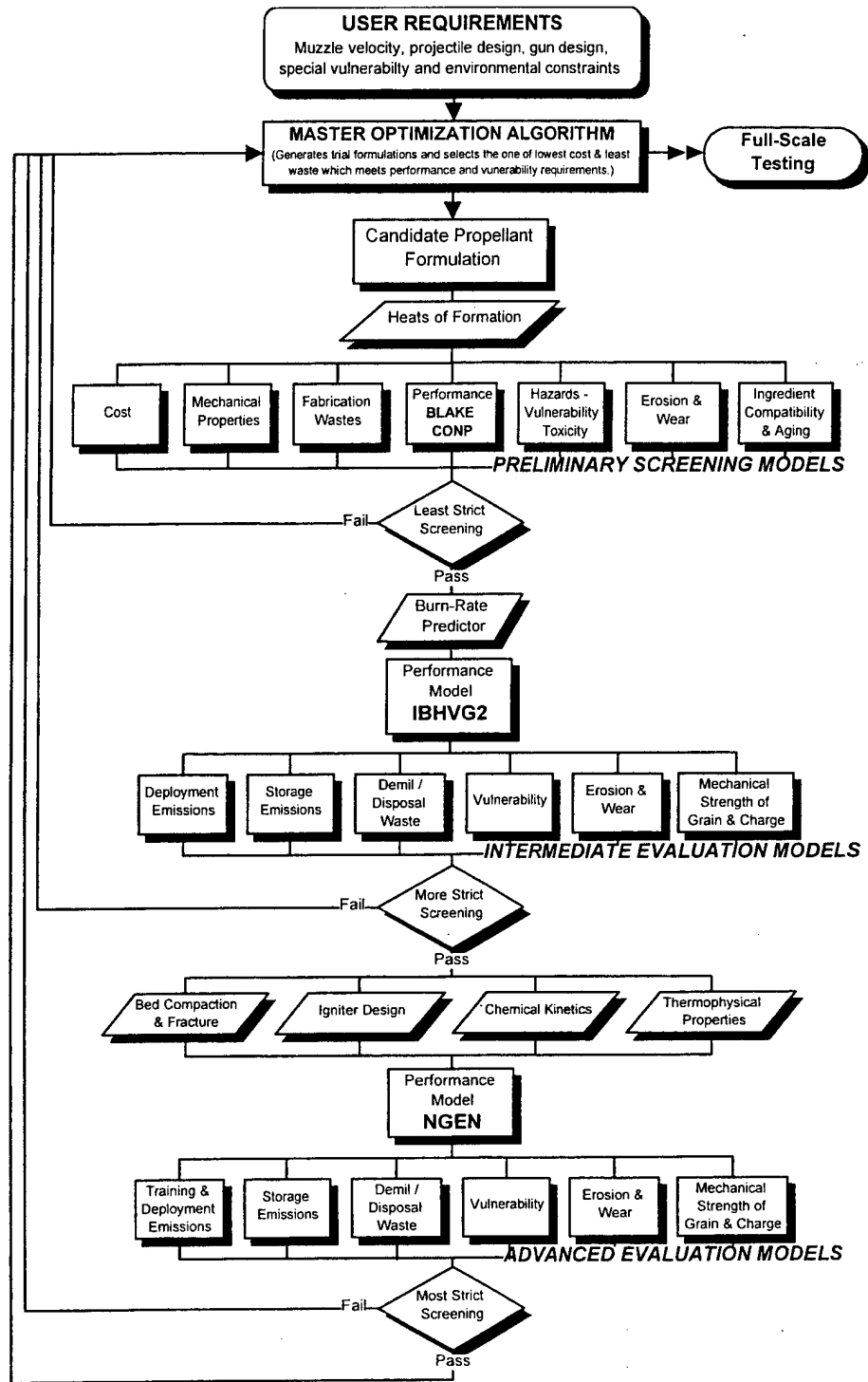


Figure 4. Flow Chart Illustrating the Progressive Wining of Propellant Candidates Through a Hierarchy of Models of Increasing Sophistication.

Table 4. Identification of Codes Used in Figure 4

Code	Description	Reference
BLAKE	Equilibrium thermochemistry	[13]
CONPRESS	Constant-pressure ideal gun	[14]
IBHVG2	Lumped-parameter interior ballistics	[15]
XNOVAKTC	Quasi-1-D interior ballistics with flamespreading	[8, 9]
NGEN	2-D/3-D advanced interior ballistics	[16, 17]

exercise was completely dependent on knowledge of the toxicity of the ingredients and knowledge of the combustion properties (such as burning rate, etc.) to perform the screening tests. For notional materials that might be developed for advanced propulsion concepts, this information will not be readily available, and a need exists for predictive models of such. Also, the current models do not accurately predict product emissions from the gun into the atmosphere after gun firing events, which would be an important factor in an environmentally driven development procedure. The most that current models can do is assume that the combustion products are in thermal equilibrium, a situation that may not exist in a gun-firing environment. This deficiency could be remedied by enhancing existing interior ballistics codes to calculate finite rate chemistry at the muzzle. The parallel demonstration also makes use of previously measured burning rates. First-principles burning rate models are under development at ARL to remove dependency on closed-bomb and strand-burner measurements, which requires fabricating any new propellant and synthesizing any new ingredient. If models are developed for all of the boxes in Figure 4, one could replace the first six steps of Figure 3 could be replaced by the hierarchical evaluation models of Figure 4 to achieve even higher cost savings than suggested by Table 3. This end goal is illustrated by the new charge development chart in Figure 5, where all of the models and logic of Figure 4 are represented by the box termed "Master Optimization Algorithm." Thus, Figure 5 represents the full measure of streamlining that might be achieved by fully implementing the science-based design approach. The savings in time and money implied by a comparison of Figure 5 to the traditional approach of Figure 2 is dramatic.

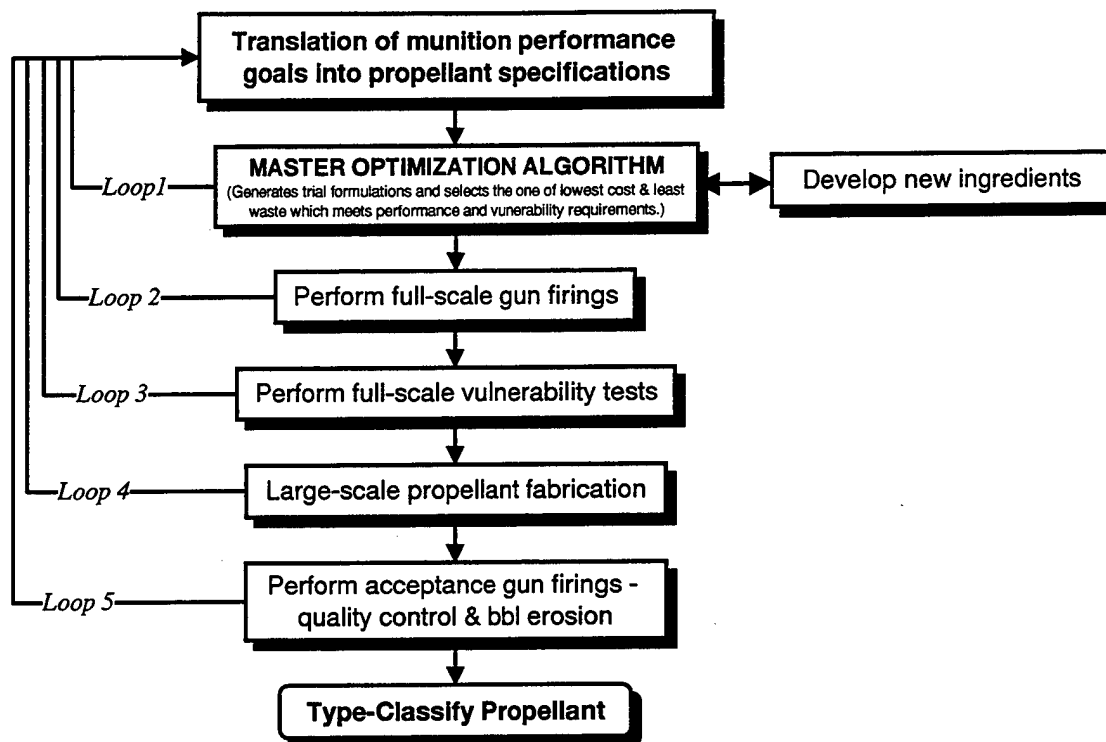


Figure 5. Simplification of Propelling-Charge Development Possible With Full Implementation of Science-Based Design (Compare to Figure 2).

This report has not discussed developing new propellant ingredients, energetic materials, and polymeric binders. It may well happen that performance objectives cannot be met with a propellant made from existing ingredients. Although represented in Figures 1–3 as a single box, there is a similar nested-loop procedure required to develop these. Ingredient development can likewise benefit from strong theoretical guidance during its early phases. Research efforts at ARL are addressing a number of relevant areas such as theoretical chemistry, detonability, and thermophysical properties of polymers. Theoretical chemistry methods can be used to predict properties of novel materials and determine whether a species is stable. These methods can also be used to guide experimental synthesis by predicting favorable reaction routes. In fact, these methods would reduce the need for chemical synthesis, a potentially costly and time-consuming step.

Implementing a science-based approach to propellant formulation will not be trivial or without its own considerable cost and delay. For example, the range of chemistry and physics involved in interior-ballistic phenomena is daunting. Interior-ballistic codes have long been under active

development at ARL. The most advanced code in use is NGEN [14, 15]. This code treats the entire interior-ballistic cycle, from the dispersal of the igniter gases, to flame spreading among the individual propellant grains that make up a propelling charge, to the motion of the projectile down the gun barrel. Descriptions of the full boundary layer flow in and between these grains is not practical, so temporal and spatial averages over this microstructure are effected using mixture theory. This approach necessitates using phenomenological correlations to describe some basic physical interactions, such as drag and heat transfer. While the current correlations seem to work well for a wide range of ballistic problems in artillery and tank weaponry, the demand for ever higher performance may expose new regimes where existing correlations or even the mixture-theory approach itself fails. Should this occur, considerable theoretical work may be required before these ballistic regimes could be modeled accurately. On the other hand, an experimental trial and error approach, in addition to being inefficient and costly, may simply fail.

A rigorous theory of isolated propellant combustion is not yet attainable, largely because of the embryonic state of the theory of reactions in the condensed phase. Even in the gas phase, where both experimental and theoretical techniques exist to treat virtually any reaction, many reactions are poorly known, and remedying these data deficiencies may prove to be both expensive and time consuming. On the other hand, we are at an opportune time in history when the maturation of powerful scientific tools (such as density-functional theory for computing quantum structure of large molecules, molecular dynamics with realistic force fields, and unprecedented computer resources) give confidence to an optimistic prognosis for achieving these goals.

Developing models to fill the screening and evaluation boxes in Figure 4 represents a very great scientific challenge. However, a technically sound and systematic approach to developing the needed models should lead inexorably toward the ultimate goal and provide valuable partial guidance along the way. In any event, the simple simulations presented in this report underscore the unworkability of applying the traditional trial-and-error development approach with the added burden of considering life-cycle costs. Employing modeling and simulation to the early development phases can achieve impressive reductions in cost and time. In view of the national need to provide ever stronger

weapons capabilities in the face of declining resources, there appears to be little choice but to pursue a science-based strategy to minimizing these life-cycle costs. Again echoing the words of the Quadrennial Review, "We not only have the opportunity to change, we have the requirement to change."

INTENTIONALLY LEFT BLANK.

6. References

1. Cohen, W. S. "Report of the Quadrennial Defense Review." Department of Defense, Washington, DC, May 1997.
2. Shalikashvili, J. M. "Joint Vision 2010." Office of the Chairman of the Joint Chiefs of Staff, Pentagon, Washington, DC, November 1996.
3. Short, J., and H. Bright. "Green Energetics." Strategic Environmental Research and Development Program (SERDP) In-Process Review, Arlington, VA, 11 May 1999.
4. Merwin, L. "Solventless Manufacture of Artillery Propellant Using Thermoplastic Elastomer Binder." Strategic Environmental Research and Development Program (SERDP) In-Process Review, Arlington, VA, 11 May 1999.
5. Sorescu, D. C., B. M. Rice, and D. L. Thompson. "Molecular Packing and NPT-Molecular Dynamics Investigation of the Transferability of the RDX Intermolecular Potential to 2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane." *Journal of Physical Chemistry B*, vol. 102, p. 948, 1998.
6. Sorescu, D. C., B. M. Rice, and D. L. Thompson. "A Transferable Intermolecular Potential for Nitramine Crystals." *Journal of Physical Chemistry A*, vol. 102, p. 8386, 1998.
7. Sorescu, D. C., B. M. Rice, and D. L. Thompson. "A Molecular Packing and Molecular Dynamics Study of the Transferability of a Generalized Nitramine Intermolecular Potential to Non-Nitramine Crystals." *Journal of Physical Chemistry A*, vol. 103, p. 989, 1999.
8. Rice, B. M., S. V. Pai, and J. Hare. "Predicting Heats of Formation of Energetic Materials Using Quantum Mechanical Calculations." *Combustion and Flame*, to be published.
9. Miller, M. S., and W. R. Anderson. "Energetic-Material Combustion Modeling With Elementary Gas-Phase Reactions: A Practical Approach." *Journal of Propulsion and Power*, to be published.
10. Kooker, D. E., and A. J. Kotlar. "Predicting Convective Ignition Delay of Solid Propellant Based on Flame Zone Chemical Decomposition Schemes." 34th JANNAF Combustion Subcommittee Meeting, *CPIA Publication 662*, vol. 1, pp. 163-180, October 1997.
11. Gough, P. S. "Improvements to the XNOVAKTC and TDNOVA Codes." BRL-CR-233, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, June 1995.

12. Anderson, R. D., and B. M. Rice. "Minimizing Life-Cycle Costs of Gun Propellant Selection Through Model-Based Decision Making: A Case Study in Environmental Screening and Performance Testing." U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, to be published.
13. Freedman, E. "BLAKE—A Thermodynamics Code Based on TIGER: User's Guide to the Revised Program." ARL-CR-422, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, July 1998.
14. Oberle, W. F. "Constant Pressure Interior Ballistics Code CONPRESS: Theory and User's Manual." ARL-TR-199, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, September 1993.
15. Anderson, R. D., and K. D. Fickie. "IBHVG2 - A User's Guide." BRL-TR-2829, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1987.
16. Gough, P. S. "Formulation of a Next-Generation Interior Ballistic Code." ARL-CR-68, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, September 1993.
17. Nusca, M. J., and P. S. Gough. "Numerical Model of Multiphase Flows Applied to Solid Propellant Combustion in Gun Systems." 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, *AIAA Paper 98-3695*, July 1998.

NO. OF
COPIES ORGANIZATION

2 DEFENSE TECHNICAL
INFORMATION CENTER
DTIC DDA
8725 JOHN J KINGMAN RD
STE 0944
FT BELVOIR VA 22060-6218

1 HQDA
DAMO FDT
400 ARMY PENTAGON
WASHINGTON DC 20310-0460

1 OSD
OUSD(A&T)/ODDDR&E(R)
R J TREW
THE PENTAGON
WASHINGTON DC 20301-7100

1 DPTY CG FOR RDA
US ARMY MATERIEL CMD
AMCRDA
5001 EISENHOWER AVE
ALEXANDRIA VA 22333-0001

1 INST FOR ADVNCD TCHNLGY
THE UNIV OF TEXAS AT AUSTIN
PO BOX 202797
AUSTIN TX 78720-2797

1 DARPA
B KASPAR
3701 N FAIRFAX DR
ARLINGTON VA 22203-1714

1 NAVAL SURFACE WARFARE CTR
CODE B07 J PENNELLA
17320 DAHLGREN RD
BLDG 1470 RM 1101
DAHLGREN VA 22448-5100

1 US MILITARY ACADEMY
MATH SCI CTR OF EXCELLENCE
DEPT OF MATHEMATICAL SCI
MADN MATH
THAYER HALL
WEST POINT NY 10996-1786

NO. OF
COPIES ORGANIZATION

1 DIRECTOR
US ARMY RESEARCH LAB
AMSRL D
D R SMITH
2800 POWDER MILL RD
ADELPHI MD 20783-1197

1 DIRECTOR
US ARMY RESEARCH LAB
AMSRL DD
2800 POWDER MILL RD
ADELPHI MD 20783-1197

1 DIRECTOR
US ARMY RESEARCH LAB
AMSRL CS AS (RECORDS MGMT)
2800 POWDER MILL RD
ADELPHI MD 20783-1145

3 DIRECTOR
US ARMY RESEARCH LAB
AMSRL CI LL
2800 POWDER MILL RD
ADELPHI MD 20783-1145

ABERDEEN PROVING GROUND

4 DIR USARL
AMSRL CI LP (BLDG 305)

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
3	COMMANDER US ARMY RESEARCH OFFICE D MANN R SINGLETON R SHAW PO BOX 12211 RESEARCH TRIANGLE PARK NC 27709-2211
1	DIRECTOR ARMY RESEARCH OFFICE AMXRO RT IP LIBRARY SERVICES PO BOX 12211 RESEARCH TRIANGLE PARK NC 27709-2211
4	COMMANDER US ARMY ARDEC AMSTA AR AEE B C CAPELLOS D S DOWNS L HARRIS T VLADIMIROV PICATINNY ARSENAL NJ 07806-5000
1	COMMANDER US ARMY ARDEC AMSTA AR AEE R PRICE PICATINNY ARSENAL NJ 07806-5000
2	COMMANDER US ARMY ARDEC AMSTA AR AEE J A LANNON PICATINNY ARSENAL NJ 07806-5000
2	COMMANDER US ARMY MISSILE COMMAND AMSMI RD PR E A R MAYKUT AMSMI RD PR P R BETTS REDSTONE ARSENAL HUNTSVILLE AL 35816

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	OFFICE OF NAVAL RESEARCH DEPT OF THE NAVY R S MILLER CODE 432 800 N QUINCY STREET ARLINGTON VA 22217
1	COMMANDER NAVAL AIR SYSTEMS COMMAND J RAMNARACE AIR 54111C WASHINGTON DC 20360
2	COMMANDER NAVAL SURFACE WARFARE CENTER R BERNECKER R 13 G B WILMOT R 16 SILVER SPRING MD 20903-5000
4	COMMANDER NAVAL RESEARCH LAB J MCDONALD E ORAN J SHNUR R J DOYLE CODE 6110 WASHINGTON DC 20375
2	COMMANDER NAVAL WEAPONS CENTER T BOGGS CODE 388 T PARR CODE 3895 CHINA LAKE CA 93555-6001
1	SUPERINTENDENT NAVAL POSTGRADUATE SCHOOL DEPT OF AERONAUTICS D W NETZER MONTEREY CA 93940
3	AL/LSCF R CORLEY R GEISLER J LEVINE EDWARDS AFB CA 93523-5000
1	AFOSR BOLLING AIR FORCE BASE J M TISHKOFF WASHINGTON DC 20332

NO. OF
COPIES ORGANIZATION

1 OSD/SDIO/IST
L CAVENY
PENTAGON
WASHINGTON DC 20301-7100

1 COMMANDANT
USAFAS
ATSF TSM CN
FORT SILL OK 73503-5600

1 UNIV OF DAYTON RSRCH INSTITUTE
D CAMPBELL
AL/PAP
EDWARDS AFB CA 93523

1 NASA
LANGLEY RESEARCH CENTER
LANGLEY STATION
G B NORTHAM MS 168
HAMPTON VA 23365

4 NATIONAL BUREAU OF STANDARDS
US DEPARTMENT OF COMMERCE
J HASTIE
M JACOX
T KASHIWAGI
H SEMERJIAN
WASHINGTON DC 20234

2 DIRECTOR
LAWRENCE LIVERMORE NATL LAB
C WESTBROOK
W TAO MS L 282
PO BOX 808
LIVERMORE CA 94550

1 DIRECTOR
LOS ALAMOS NATIONAL LAB
B NICHOLS T7 MS B284
PO BOX 1663
LOS ALAMOS NM 87545

1 PRINCETON COMBUSTION
RESEARCH LABORATORIES INC
N A MESSINA
PRINCETON CORPORATE PLAZA
BLDG IV SUITE 119
11 DEERPARK DRIVE
MONMOUTH JUNCTION NJ 08852

NO. OF
COPIES ORGANIZATION

3 DIRECTOR
SANDIA NATIONAL LAB
DIVISION 8354
R BEHRENS
W MCLEAN
C MELIUS
LIVERMORE CA 94550

1 BRIGHAM YOUNG UNIVERSITY
DEPT OF CHEMICAL ENGINEERING
M W BECKSTEAD
PROVO UT 84058

1 CALIF INSTITUTE OF TECH
JET PROPULSION LABORATORY
L STRAND MS 125 224
4800 OAK GROVE DR
PASADENA CA 91109

1 CALIF INSTITUTE OF TECH
FEC CULIC MC 301 46
204 KARMAN LAB
PASADENA CA 91125

1 UNIVERSITY OF CALIF
LOS ALAMOS SCIENTIFIC LAB
PO BOX 1663 MAIL STOP B216
LOS ALAMOS NM 87545

1 UNIV OF CALIF BERKELEY
CHEMISTRY DEPT
C BRADLEY MOORE
211 LEWIS HALL
BERKELEY CA 94720

1 UNIV OF CALIF SAN DIEGO
F A WILLIAMS
AMES B010
LA JOLLA CA 92093

2 UNIV OF CALIF SANTA BARBARA
QUANTUM INSTITUTE
K SCHOFIELD
M STEINBERG
SANTA BARBARA CA 93106

NO. OF COPIES	ORGANIZATION
1	UNIV OF COLORADO BOULDER ENGINEERING CENTER J DAILY CAMPUS BOX 427 BOULDER CO 80309-0427
3	UNIV OF SOUTHERN CALIF DEPT OF CHEMISTRY R BEAUDET S BENSON C WITTIG LOS ANGELES CA 90007
1	CORNELL UNIVERSITY DEPT OF CHEMISTRY T A COOL BAKER LABORATORY ITHACA NY 14853
1	UNIVERSITY OF DELAWARE T BRILL CHEMISTRY DEPT NEWARK DE 19711
1	UNIVERSITY OF FLORIDA DEPT OF CHEMISTRY J WINEFORDNER GAINESVILLE FL 32611
3	GEORGIA INST OF TECH SCHOOL OF AEROSPACE ENGNRG E PRICE W C STRAHLE B T ZINN ATLANTA GA 30332
2	UNIVERSITY OF ILLINOIS DEPT OF MECH ENG H KRIER Q BREWSTER 144 MEB 1206 W GREEN ST URBANA IL 61801

NO. OF COPIES	ORGANIZATION
1	THE JOHNS HOPKINS UNIVERSITY CHEMICAL PROPULSION INFORMATION AGENCY T W CHRISTIAN 10630 LITTLE PATUXENT PARKWAY SUITE 202 COLUMBIA MD 21044-3200
1	UNIVERSITY OF MICHIGAN GAS DYNAMICS LAB AEROSPACE ENGINEERING BLDG G M FAETH ANN ARBOR MI 48109-2140
1	UNIVERSITY OF MINNESOTA DEPT OF MECHANICAL ENGINEERING E FLETCHER MINNEAPOLIS MN 55455
4	PENN STATE UNIVERSITY DEPT OF MECHANICAL ENGNRG K KUO M MICCI S THYNELL V YANG UNIVERSITY PARK PA 16802
2	PRINCETON UNIVERSITY FORRESTAL CAMPUS LIBRARY K BREZINSKY I GLASSMAN PO BOX 710 PRINCETON NJ 08540
1	PURDUE UNIVERSITY SCHOOL OF AERONAUTICS AND ASTRONAUTICS GRISSOM HALL J R OSBORN WEST LAFAYETTE IN 47906
1	PURDUE UNIVERSITY DEPT OF CHEMISTRY E GRANT WEST LAFAYETTE IN 47906

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
2	PURDUE UNIVERSITY SCHOOL OF MECHANICAL ENGNRG TSPC CHAFFEE HALL N M LAURENDEAU S N B MURTHY WEST LAFAYETTE IN 47906
1	RENSSELAER POLYTECHNIC INST DEPT OF CHEMICAL ENGINEERING A FONTIJN TROY NY 12181
1	STANFORD UNIVERSITY DEPT OF MECHANICAL ENGNRG R HANSON STANFORD CA 94305
1	UNIVERSITY OF TEXAS DEPT OF CHEMISTRY W GARDINER AUSTIN TX 78712
1	VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY J A SCHETZ BLACKSBURG VA 24061
1	APPLIED COMBUSTION TECH INC A M VARNEY PO BOX 607885 ORLANDO FL 32860
2	APPLIED MECHANICS REVIEWS THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS R E WHITE A B WENZEL 345 E 47TH STREET NEW YORK NY 10017
1	TEXTRON DEFENSE SYSTEMS A PATRICK 2385 REVERE BEACH PARKWAY EVERETT MA 02149-5900
1	BATTELLE TWSTIA C HUGGINS 505 KING AVENUE COLUMBUS OH 43201-2693

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	COHEN PROFESSIONAL SERVICES N S COHEN 141 CHANNING STREET REDLANDS CA 92373
1	EXXON RESEARCH & ENG CO A DEAN ROUTE 22E ANNANDALE NJ 08801
1	GENERAL APPLIED SCIENCE LAB INC 77 RAYNOR AVENUE RONKONKAMA NY 11779-6649
1	GEN ELEC ORDNANCE SYSTEMS J MANDZY 100 PLASTICS AVENUE PITTSFIELD MA 01203
1	GENERAL MOTORS RSRCH LABS PHYSICAL CHEMISTRY DEPT T SLOANE WARREN MI 48090-9055
2	HERCULES INC ALLEGHENY BALLISTICS LAB W B WALKUP E A YOUNT PO BOX 210 ROCKET CENTER WV 26726
1	HERCULES INC R V CARTWRIGHT 100 HOWARD BLVD KENVIL NJ 07847
1	ALLIANT TECHSYSTEMS INC MARINE SYSTEMS GROUP D E BRODEN MS MN50 2000 600 SECOND STREET NE HOPKINS MN 55343
1	ALLIANT TECHSYSTEMS INC R E TOMPKINS MN 11 2720 600 SECOND ST NE HOPKINS MN 55343

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	IBM CORPORATION A C TAM RESEARCH DIVISION 5600 COTTLE ROAD SAN JOSE CA 95193
1	IIT RESEARCH INSTITUTE R F REMALY 10 WEST 35TH STREET CHICAGO IL 60616
1	LOCKHEED MISSILES & SPACE CO G LO 3251 HANOVER STREET DEPT 52 35 B204 2 PALO ALTO CA 94304
1	OLIN ORDNANCE V MCDONALD LIBRARY PO BOX 222 ST MARKS FL 32355-0222
1	PAUL GOUGH ASSOCIATES INC P S GOUGH 1048 SOUTH STREET PORTSMOUTH NH 03801-5423
1	HUGHES AIRCRAFT COMPANY T E WARD 8433 FALLBROOK AVENUE CANOGA PARK CA 91303
1	ROCKWELL INTERNATIONAL CORP ROCKETDYNE DIVISION J E FLANAGAN HB02 6633 CANOGA AVENUE CANOGA PARK CA 91304
1	SCIENCE APPLICATIONS INC R B EDELMAN 23146 CUMORAH CREST WOODLAND HILLS CA 91364
3	SRI INTERNATIONAL G SMITH D CROSLEY D GOLDEN 333 RAVENSWOOD AVENUE MENLO PARK CA 94025

<u>NO. OF COPIES</u>	<u>ORGANIZATION</u>
1	STEVENS INSTITUTE OF TECH DAVIDSON LABORATORY R MCALEVY III HOBOKEN NJ 07030
1	SVERDRUP TECHNOLOGY INC LERC GROUP R J LOCKE MS SVR 2 2001 AEROSPACE PARKWAY BROOK PARK OH 44142
1	SVERDRUP TECHNOLOGY INC J DEUR 2001 AEROSPACE PARKWAY BROOK PARK OH 44142
3	THIOKOL CORPORATION ELKTON DIVISION TECH LIB R BIDDLE R WILLER PO BOX 241 ELKTON MD 21921
1	THIOKOL CORPORATION WASATCH DIVISION S J BENNETT PO BOX 524 BRIGHAM CITY UT 84302
1	UNITED TECHNOLOGIES RSRCH CTR A C ECKBRETH EAST HARTFORD CT 06108
1	UNITED TECHNOLOGIES CORP CHEMICAL SYSTEMS DIVISION R R MILLER PO BOX 49028 SAN JOSE CA 95161-9028
1	UNIVERSAL PROPULSION COMPANY H J MCSPADDEN 25401 NORTH CENTRAL AVENUE PHOENIX AZ 85027-7837
1	VERITAY TECHNOLOGY INC E B FISHER 4845 MILLERSPORT HIGHWAY PO BOX 305 EAST AMHERST NY 14051-0305

NO. OF
COPIES ORGANIZATION

1 FREEDMAN ASSOCIATES
E FREEDMAN
2411 DIANA ROAD
BALTIMORE MD 21209-1525

6 ALLIANT TECHSYSTEMS
R BECKER
J BODE
R BURETTA
C CANDLAND
L OSGOOD
M SWENSON
600 SECOND ST NE
HOPKINS MN 55343

1 US ARMY BENET LABORATORY
AMSTA AR CCB B
S SOPOK
WATERVLIET NY 12189

ABERDEEN PROVING GROUND

23 DIR USARL
AMSRL WM B
A HORST
AMSRL WM BD
B E FORCH
W R ANDERSON (4 CPS)
S W BUNTE
C F CHABALOWSKI
S COLEMAN
B E HOMAN
P KASTE
A J KOTLAR
M MCQUAID
M S MILLER (4 CPS)
R A PESCE-RODRIGUEZ
P REEVES
B M RICE
R C SAUSA
M A SCHROEDER
J A VANDERHOFF

NO. OF
COPIES ORGANIZATION

INTENTIONALLY LEFT BLANK.

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE August 2000	3. REPORT TYPE AND DATES COVERED Final, 1 Jul 98 - 1 Jul 99		
4. TITLE AND SUBTITLE A New Approach to Propellant Formulation: Minimizing Life-Cycle Costs Through Science-Based Design		5. FUNDING NUMBERS 622618AH80		
6. AUTHOR(S) Martin S. Miller, Betsy M. Rice, Anthony J. Kotlar, and Randall J. Cramer*				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) U.S. Army Research Laboratory ATTN: AMSRL-WM-BD Aberdeen Proving Ground, MD 21005-5066		8. PERFORMING ORGANIZATION REPORT NUMBER ARL-TR-2291		
9. SPONSORING/MONITORING AGENCY NAMES(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER		
11. SUPPLEMENTARY NOTES * Naval Surface Warfare Center, Indian Head Division, Indian Head, MD This report is to be published in <i>Clean Products and Processes</i> .				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) The traditional approach to developing propellants for specific gun applications relies heavily on trial and error. Candidate formulations must be made in small quantities and subjected to burning-rate measurements and small-scale vulnerability assessments. If the properties of these candidates fail to meet expectations, the process must be repeated. This approach, while historically unavoidable, is obviously inefficient in time and expense and can generate considerable waste streams associated with unsuccessful formulations. With added considerations of life-cycle costs, including environmental impact at all stages of development, use, and disposal, this traditional approach becomes increasingly unworkable. This report proposes a new approach that makes maximal use of scientific understanding embodied in models during the early phases of the propellant-development cycle. Simple simulations show that this strategy can have a significant impact on the overall costs of the development process. In analogy to the Department of Energy (DOE) program to convert the nuclear-weapon stewardship from testing-based to science-based, we term the new approach science-based design. This new approach will require concentration and leveraging of resources toward the most critical early-phase development steps; with the reality of declining resources, it may be the only credible strategy to reconcile the need for higher-performance weapons.				
14. SUBJECT TERMS propellant formulation, life-cycle vests		15. NUMBER OF PAGES 35		16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL	

INTENTIONALLY LEFT BLANK.

USER EVALUATION SHEET/CHANGE OF ADDRESS

This Laboratory undertakes a continuing effort to improve the quality of the reports it publishes. Your comments/answers to the items/questions below will aid us in our efforts.

1. ARL Report Number/Author ARL-TR-2291 (Miller) Date of Report August 2000
2. Date Report Received _____
3. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which the report will be used.) _____

4. Specifically, how is the report being used? (Information source, design data, procedure, source of ideas, etc.) _____

5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided, or efficiencies achieved, etc? If so, please elaborate. _____

6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.) _____

CURRENT
ADDRESS

Organization

Name

E-mail Name

Street or P.O. Box No.

City, State, Zip Code

7. If indicating a Change of Address or Address Correction, please provide the Current or Correct address above and the Old or Incorrect address below.

OLD
ADDRESS

Organization

Name

Street or P.O. Box No.

City, State, Zip Code

(Remove this sheet, fold as indicated, tape closed, and mail.)
(DO NOT STAPLE)

DEPARTMENT OF THE ARMY

OFFICIAL BUSINESS

BUSINESS REPLY MAIL

FIRST CLASS PERMIT NO 0001,APG,MD

POSTAGE WILL BE PAID BY ADDRESSEE

DIRECTOR
US ARMY RESEARCH LABORATORY
ATTN AMSRL WM BD
ABERDEEN PROVING GROUND MD 21005-5066



NO POSTAGE
NECESSARY
IF MAILED
IN THE
UNITED STATES

